Stochastic modelling of the geometrical variability in textile composites using experimental data

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Abstract

Realistic descriptions of a carbon-epoxy 2/2 twill woven composite are generated by a stochastic multi-scale modelling approach. First, experimental data are collected on the short- and long-range variations in the reinforcement structure. Statistical information of each tow path parameter is computed in terms of mean, standard deviation and correlation information. Next, virtual reinforcements are constructed as a combination of average trends with zero-mean deviations. Depending on the presence of cross-correlation, either the Monte Carlo Markov Chain algorithm or a cross-correlated Series Expansion is applied to generate the random tow path deviations. The stochastic tow path instances are subsequently used to construct virtual composite specimens in the WiseTex format. Each specimen possesses the statistical data of the experimental samples on average.

1 Introduction

The internal architecture of textile composites is subjected to a significant amount of variability. Though, composite components are frequently modelled as identical repetitive unit cells with regular tow path descriptions. Scatter in the geometry is often not considered resulting in unreliable predictions of performance. A complete characterisation of the spatial geometrical fluctuations of the textile composite improves the quality of numerical analyses and permits to quantify the effect of reinforcement variability on the macro-scale properties.

When constructing such realistic representations, it is important to support the simulation procedure with statistical information derived from experimental data. The simulation strategy of Charmpis et al. [1] describes the construction of virtual specimens as a two-step procedure: (i) collection of sufficient experimental data on the uncertain spatially correlated geometrical characteristics on the short- and long-range, and (ii) derivation probabilistic information for the macroscopic mechanical properties from the lower scale mechanical characteristics.

This paper presents the general approach and successive steps to build random virtual specimens of a 2/2 twill woven carbon fibre reinforced epoxy composite. Measured tow path variations are reproduced by two different geometry generator techniques. Tow parameters which are only correlated along their path are simulated by the Monte Carlo Markov Chain method [2]. When a tow property is correlated along and between neighbouring tow paths, a framework based on a cross-correlated Series Expansion is chosen [3]. The objectives of the paper are to (i) propose a stochastic multi-scale framework, (ii) derive statistical information on the short- and long-range distance from experimental samples, (iii) generate zero-mean deviations using appropriate generator algorithms and (iv) construct a macro-scale random virtual specimen in the WiseTex software.

2 Stochastic multi-scale framework

Realistic descriptions of the internal geometry of textile composites are obtained by subsequently following three steps:

1. **Collection of experimental data with statistical analysis**
   (a) Quantification of the short-range variation
   (b) Quantification of the long-range variation
   (c) Statistical analysis in terms of average trends, standard deviation and correlation information
2. **Stochastic multi-scale modelling of the reinforcement**
   (a) Combination of systematic and handling trends from the experimental data
   (b) Monte Carlo Markov Chain method for simulating auto-correlated deviations
   (c) Cross-correlated Series Expansion for simulating auto- & cross-correlated deviations
3. **Construction of virtual specimens in the WiseTex software**
   (a) Construction of the nominal model with manufacturer's data
   (b) Update tow path descriptions with generated instances

3 Collection of experimental data with statistical analysis

The developed methodology is demonstrated for a 2/2 twill woven composite. The dry reinforcement is a fabric from Hexcel (G0986) [5] which is impregnated with epoxy in a Resin Transfer Moulding (RTM) process. It is a balanced textile with four warp (x-axis) and four weft (y-axis) tows. A virtual representation of the unit cell is given in figure 1 with λ_x=11.43 mm and λ_y=11.43 mm, respectively the periodic lengths of warp and weft tows.

The full tow path is characterised on the short- and long-range for the centroid coordinates (x, y, z), tow aspect ratio AR and tow area A. Considering the production process of the 2/2 twill woven fabric, warp

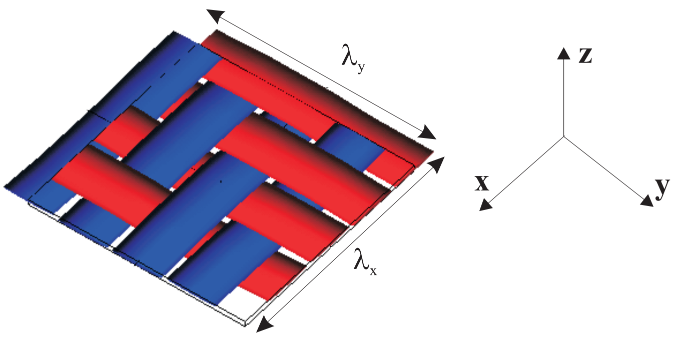

Figure 1: WiseTex model of a 2/2 twill woven reinforcement. The x-axis and y-axis of the coordinate system are respectively parallel to the warp and weft direction.

tows can be represented by one representative tow, called *genus*, and similar for the weft tows. The statistical information is quantified in terms of average trends, standard deviation and correlation information. Correlation is investigated along a single tow, called *auto-correlation*, and between neighbouring tows of the same genus, named *cross-correlation*.

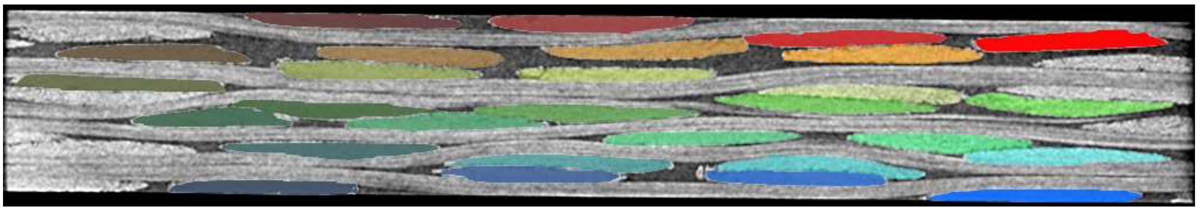

Figure 2: Digital image of a cross-section in weft direction, extracted from the reconstructed volume obtained by micro-CT. The segmented tows have an elliptical shape.

Short-range data on uncertain tow path parameters are identified in [7] from a seven-ply unit cell sample using micro-CT. A three-dimensional (3-D) reconstructed volume is obtained, wherefrom two-dimensional (2-D) slices are extracted in warp and weft direction. Nineteen equidistant slices are considered to analyse the entire tow path, with figure 2 showing such a cross-section. After the collection of geometrical data, the reference period collation method [6] is applied, where each tow parameter is decomposed in a non-stochastic, periodic systematic trend and non-periodic stochastic fluctuations. All tow parameters, with exception of the in-plane centroid position, vary within the unit cell dimensions. This is indicated by the correlation length ξ which exceeds the unit cell dimensions for the in-plane position. The latter centroid position is also subjected to the largest variability, indicated by the high standard deviation σ, and is found to be cross-correlated between neighbouring tows [8]. The micro-CT procedure and derived statistical information is described in [7].

Additional long-range information about the in-plane centroid positions is acquired from larger samples. An optical scan of the in-plane dimension of a single-ply composite, spanning 13 by 13 unit cells, is performed. A region of 10 by 10 unit cells is inspected wherein the in-plane tow data are analysed. This area of interest is chosen away from the edges to minimise possible edge effects and large enough, roughly one magnitude larger than the short range data. The in-plane centreline of each tow is extracted using image processing tools. Next, in-plane warp and weft undulations are considered respectively in y- and x-direction, and decomposed in a non-periodic handling trend and zero-mean deviations. The statistical analysis demonstrates that the weft tows have a standard deviation which is six times higher compared to the warp direction. Correlation along the tow path is found to be twice as high for the warp tows, around ten unit cells, while the correlation between different tows is much higher for the weft tows with a distance exceeding the unit cell size. A detailed discussion of the procedure and results are given in [9].

	x [mm]	**y [mm]**	**z [mm]**	AR **[-]**	A **[mm^2]**
σ^{warp} [mm]	-	0.106	0.014	1.774	0.023
ξ^{warp}_{auto} [mm]	-	114.89	1.78	7.26	2.53
ξ^{warp}_{cross} [mm]	-	4.49	-	-	-
σ^{weft} [mm]	0.615	-	0.015	1.440	0.024
ξ^{weft}_{auto} [mm]	52.89	-	1.62	5.48	1.01
ξ^{weft}_{cross} [mm]	13.16	-	-	-	-

Table 1: Statistical information of all tow path parameters: standard deviation, auto- and cross-correlation length.

The short- and long-range statistical information of all tow path parameters are used as input to simulate virtual textile composites. All deviations are approximately represented by a normal distribution, with a summary of the statistical data given in table 3. Only the in-plane centroid position is cross-correlated between neighbouring tows.

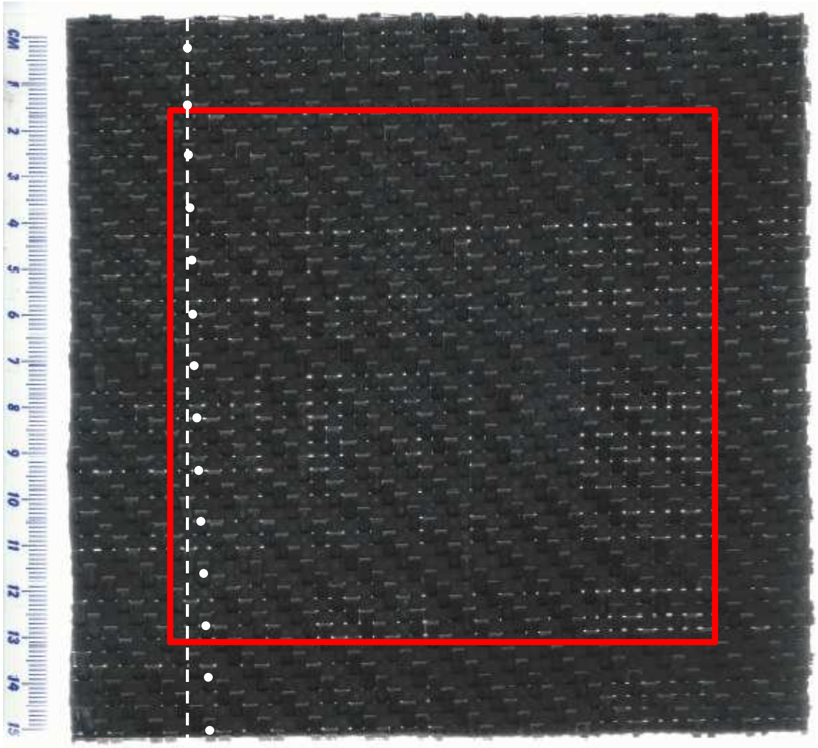

Figure 3: Digital image of a single ply 2/2 twill woven carbon-epoxy composite. Warp and weft tows are respectively positioned horizontally and vertically. The red square indicates the region where the in-plane position is quantified.

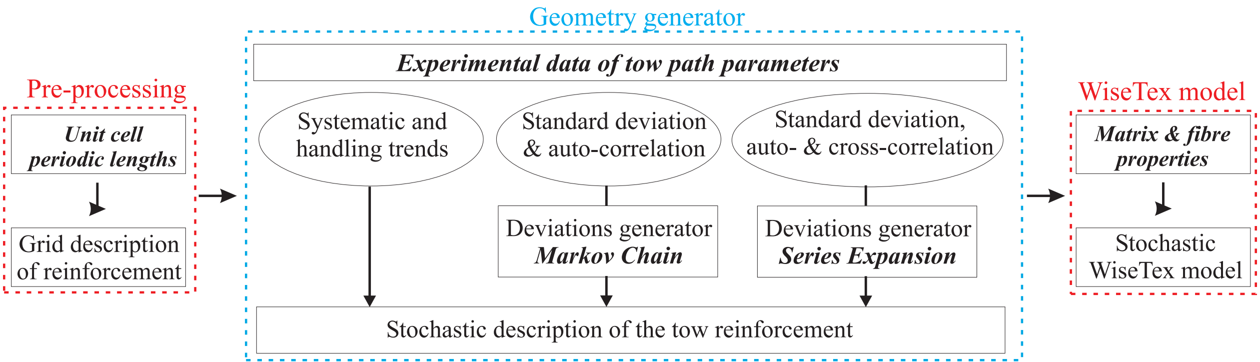

Figure 4: Stochastic multi-scale modelling approach.

4 Stochastic multi-scale modelling of the reinforcement

Virtual textile specimens spanning ten by ten unit cells are generated using the approach presented in figure 4. First, a 2-D lattice with equidistant grid is constructed with rows indicating the warp direction and columns representing the weft direction. The length of this grid in x- and y-direction is equal to ten times the experimentally derived unit cell dimensions. Secondly, the systematic and handling trends of all tow path parameters, determined from experiments, are added to this lattice to obtain an average representation. In a third and fourth step, zero-mean deviations are added to the average trends to obtain a random model. These fluctuations are generated using two different geometry generator principles. Tow path parameters varying within the unit cell size with no cross-correlation (out-of-plane centroid z, tow area A and tow aspect ratio AR) are generated using a Monte Carlo Markov Chain method for textile structures [2]. The cross-correlated in-plane centroid deviations are described as Gaussian random fields using a methodology

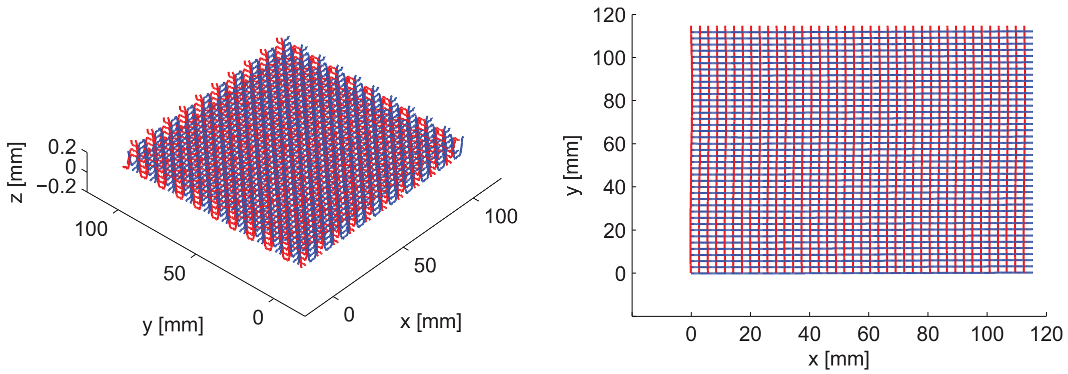

Figure 5: The average reinforcement description of a 2/2 twill woven composite.

developed by Vořechovský [3]. A virtual composite model with random geometry is obtained in the WiseTex format [4] by updating the nominal tow path description with these generated tow realisations.

4.1 Combination of systematic and handling trends from the experimental data

The average description of each tow parameter can be periodic, as expected from the concept of a unit cell, or non-periodic caused by the handling of the dry fabric before production. From the experiments, it is observed that the tow properties varying on the short-range (z, A and AR) possess a systematic periodic trend in both warp and weft direction [7], while the in-plane centroid position (y for warp tows and x for weft tows) fluctuates with non-periodic wavelengths exceeding the unit cell dimension [9]. Combination of these periodic and handling trends defines the average reinforcement of the 2/2 twill woven composite given in figure 5.

4.2 Generation of auto-correlated tow parameters

Tow path parameters which vary without any type of cross-correlation are generated using the Markov Chain algorithm for textile structures [2]. Deviations of a single tow path parameter are produced independently from other tow parameters at the same location or parameter values at neighbouring tows. In this Markov Chain method, a probability transition matrix is constructed that defines the next grid value based on the present deviation value. Each tow parameter has a different transition matrix that is calibrated with the

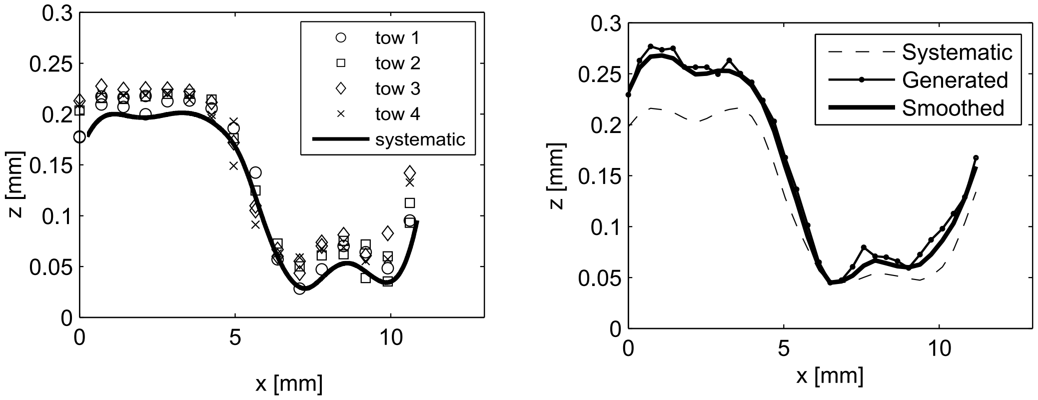

Figure 6: The warp out-of-plane tow centroid position for a single unit cell, from micro-CT (left) and generated (right) using the Markov Chain procedure. The smoothing operation removes the unphysical spikes present in the path.

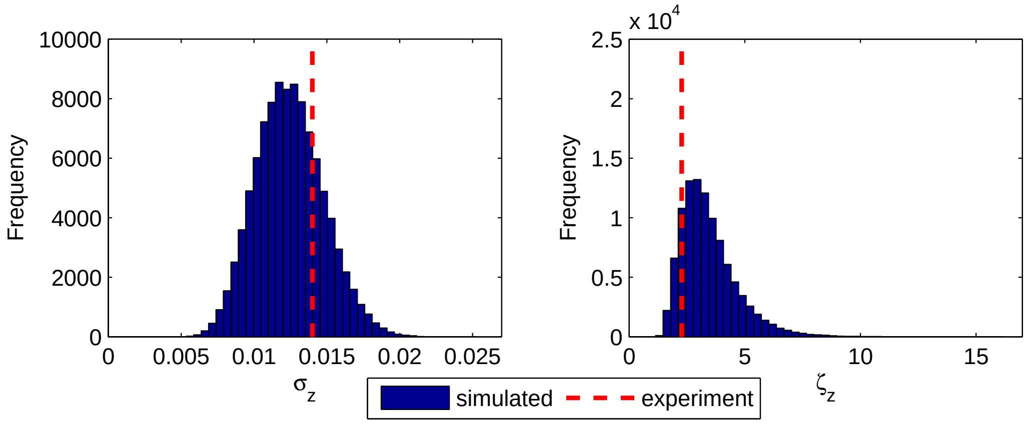

Figure 7: Unit cell standard deviations and correlation lengths of the out-of-plane warp centroid after smoothing.

experimental standard deviation and nearest-neighbour correlation information to reproduce the statistical information. A post-processing smoothing operation is required to reduce low-amplitude short-range spikes present in the discretized tow path.

This method is already successfully employed for the generation of random unit cell structures in [8], and now used to simulate the out-of-plane centroid z, area A and aspect ratio AR deviations of larger specimens. Smoothing is applied using information of ± 2 neighbouring grid points to obtain a realistic tow path, as demonstrated for the warp out-of-plane centroid for a single unit cell in figure 6.

	σ_z [mm]	σ_{AR} [-]	σ_A [mm^2]	ξ_z [mm]	ξ_{AR} [mm]	ξ_A [mm]
Target - *overall data set*	0.014	1.774	0.023	1.78	7.26	2.53
Warp tows - *with smoothing*	0.013	1.755	0.023	3.65	10.86	4.56
<Target> - *mean of unit cells* [7]	0.014	1.774	0.023	2.27	6.84	1.70
<Warp tows>- *with smoothing*	0.013	1.540	0.021	3.45	11.82	4.54

Table 2: Standard deviation and auto-correlation length of warp deviations produced with the Markov Chain algorithm for the (i) overall data set and (ii) average values for the unit cells data set.

Tow path deviations for thousand virtual specimens are generated to verify if the experimental statistics are reproduced. Table 4.2 presents the standard deviation and auto-correlation lengths for (i) the overall data set, combining the deviation values of all virtual specimens, and for (ii) the data set of individual unit cells. The statistical information of the overall data set demonstrates that the standard deviations of all parameters are simulated with high accuracy, while the correlation length of the out-of-plane centroid and tow area show significant differences from the target values. This is a result of only considering the nearest-neighbour correlation information in the procedure, and the smoothing operation. However, the same order of magnitude in correlation length is obtained. The standard deviations and auto-correlation lengths of single unit cells are centred around the experimental target values. Figure 7 shows the histogram of the unit cell statistics for the z-centroid of the warp tows. Smoothing has a limited effect on the standard deviation, while the correlation lengths are slightly shifted to higher values. Similar conclusions are made for the other tow parameters as presented in table 4.2 for the warp genus.

4.3 Generation of auto- & cross-correlated tow parameters

A methodology proposed by Vořechovský [3] is suitable to simulate tow path parameters which are correlated along the tow path and between neighbouring tows. Each uncertain parameter is represented by a Gaussian random field H_i. Realisations of this field are generated by a cross-correlated Series Expansion technique based on the Karhunen-Loève decomposition. Tows belonging to the same genus possess an identical auto-correlation structure and are at the same time cross-correlated with neighbouring tows of the same type by introducing cross-correlated random variables. This methodology requires that all parameter deviations are produced simultaneously for all tows of the same genus. The experimental statistical information is almost perfectly reproduced since the full auto- and cross-correlation structure for all point spacings is considered for the calibration step. Different realisations of the random field are acquired by the following equation:

$$H_i(x,\theta) \approx \hat{H}_i(x,\theta) = \sum_{j=1}^{N_A} \lambda_j^A \chi_{i,j}^D \phi_j^A(x) \tag{1}$$

with λ_A and ϕ_A the eigenvalues and eigenvectors of the auto-correlation structure and χ_i^D the cross-correlated random variables belonging to the field H_i. Random fields of the in-plane centroids of warp and weft tows are simulated as a truncated series. Only the largest eigenvalues and corresponding eigenvectors are considered in the procedure. The error introduced by the reduction is fixed to maximum 0.9975, meaning that 99.75% of the variability is captured.

All cross-correlated in-plane centroid deviations of the 2/2 twill woven composite are generated with this method. The produced deviation patterns along the tow path show good resemblance with the measured in-plane deviations, as shown in figure 8 for the warp tows. The short wavelength of the experimental warp fluctuations and long wavelength of the measured weft deviations are reproduced without the need of an additional smoothing operation.

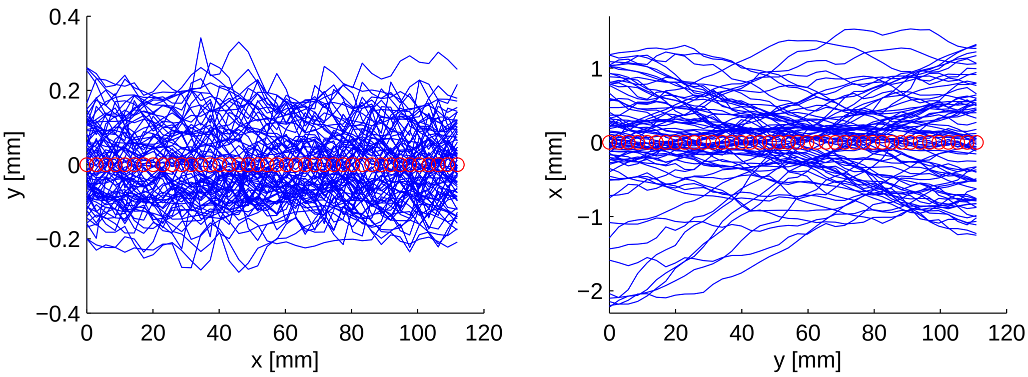

Figure 8: Comparison of experimental (left) and simulated (right) in-plane centroid deviations for 80 warp tows.

Comparison of the produced and target statistical information is performed for the (i) overall data set and the (ii) data set of the individual specimens. An overview of the statistics is given in table 4.3. The standard deviation σ and correlation lengths ξ of the overall data set demonstrate that the Series Expansion method duplicate the experimental data with high precision. The statistics at the level of individual specimens are close to the experimental values. In figure 9, the histogram is presented of the generated auto- and cross-correlation lengths for the warp tows. The mean of the generated correlation lengths achieve the target statistics on average.

	σ_{comb}	$< \sigma_{spec} >$	ξ^{auto}_{comb}	$< \xi^{auto}_{spec} >$	ξ^{cross}_{comb}	$< \xi^{cross}_{spec} >$
Target [mm]	0.106	0.106	114.89	114.89	4.49	4.49
Warp tows [mm]	0.106	0.103	115.81	114.00	4.54	4.42

Table 3: Standard deviation and correlation lengths of the in-plane warp deviations for the (i) overall data set and (ii) average values for the individual specimens.

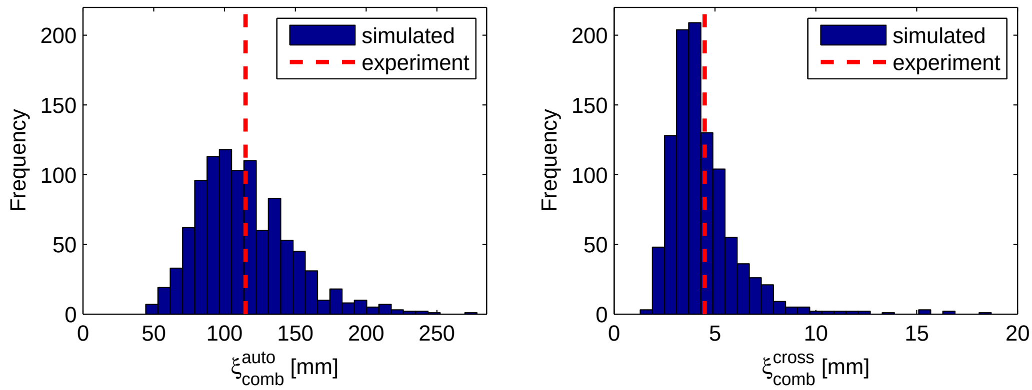

Figure 9: Auto- (left) and cross-correlation (right) lengths of produced warp in-plane positions.

5 Construction of virtual specimens in the WiseTex software

In this last step, the generated tow path instances are introduced in a nominal WiseTex model of the 2/2 twill woven composite. This idealised model is constructed using the manufacturer's data about fibre & matrix properties, and tow spacing. A stochastic representation of the internal geometry is acquired by overwriting the tow path description by the produced tow information for each specimen. Both the path length and orientation vectors that fix each cross-section of a single tow in space [8, 10] need be recomputed. This procedure is performed using the XML-structure of the WiseTex software [11].

A virtual 2/2 twill woven composite is presented in figure 10 with the warp tows oriented along the horizontal axis and the weft tows oriented along the vertical axis. The in-plane dimensional view shows the bundling behaviour of weft tows as observed in the experimental samples. Weft in-plane centroid positions are also more random along their path length, according to the statistical data of the measured geometry. On the unit cell level, both the out-of-plane centroid and the cross-sectional variations correspond to the experimental observations. However, due to the independent generation of the tow width from the in-plane position, limited interpenetration is present between neighbouring tows of the same genus. Small adaptations are thus required when transforming the WiseTex model to a finite element model.

6 Conclusions

A stochastic multi-scale framework is presented to quantify and simulate the geometrical variability present in a typical 2/2 twill woven composite. The approach consists of three general steps to acquire virtual specimens that possess the same statistical information as measured from experimental samples. In a first step, experimental data on the centroid positions and cross-sectional dimensions are collected on the short- and long-range distance. Except for the in-plane centroid position, all tow path parameters vary within unit cell dimensions. Next, virtual tow paths are constructed as combination of a mean trend with zero-mean deviations. Tow parameters without any type of cross-correlation are produced with the Monte Carlo Markov Chain method, while the cross-correlated in-plane centroid positions are generated using a cross-correlated

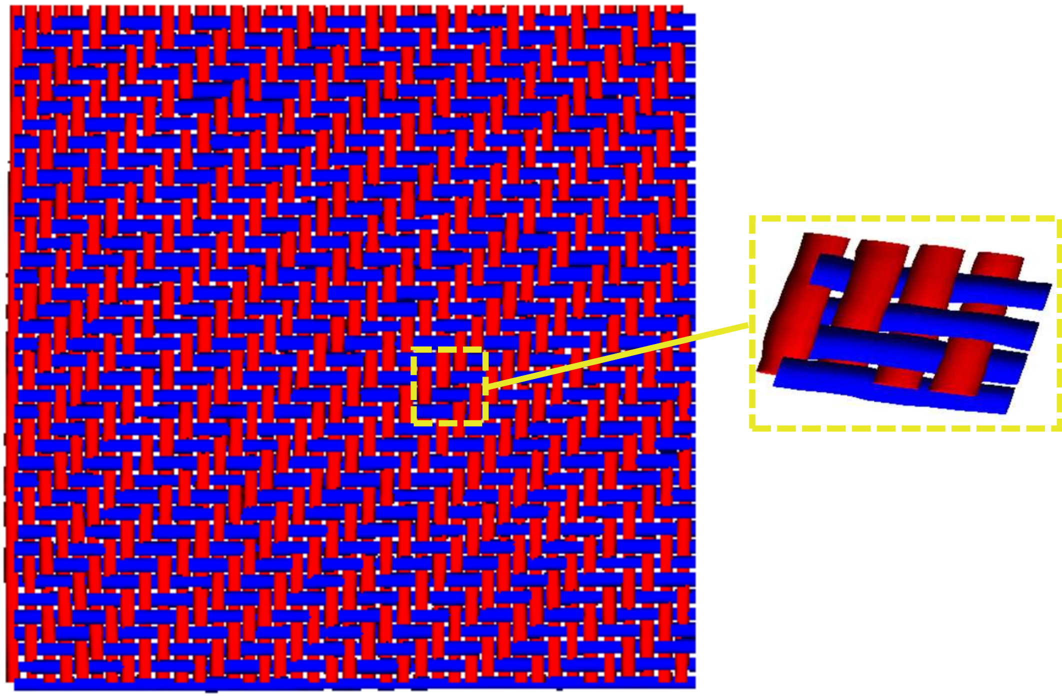

Figure 10: Virtual specimen in the WiseTex format. The in-plane dimension and a single unit cell is presented to demonstrate the short- and long-range variability.

Series Expansion technique. These random instances of reinforcement structure are used to overwrite nominal tow path descriptions of a WiseTex model to obtain realistic virtual specimens. These numerical models will support material design in predicting the mechanical performance with a higher reliability.

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